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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
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NEWS 3	NOV 26	MARPAT enhanced with FSORT command
NEWS 4	NOV 26	CHEMSAFE now available on STN Easy
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NEWS 7	DEC 12	GBFULL now offers single source for full-text coverage of complete UK patent families
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NEWS 11	FEB 02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS 12	FEB 02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS 13	FEB 06	Patent sequence location (PSL) data added to USGENE
NEWS 14	FEB 10	COMPENDEX reloaded and enhanced
NEWS 15	FEB 11	WTEXTILES reloaded and enhanced
NEWS 16	FEB 19	New patent-examiner citations in 300,000 CA/CAplus patent records provide insights into related prior art
NEWS 17	FEB 19	Increase the precision of your patent queries -- use terms from the IPC Thesaurus, Version 2009.01
NEWS 18	FEB 23	Several formats for image display and print options discontinued in USPATFULL and USPAT2
NEWS 19	FEB 23	MEDLINE now offers more precise author group fields and 2009 MeSH terms
NEWS 20	FEB 23	TOXCENTER updates mirror those of MEDLINE - more precise author group fields and 2009 MeSH terms
NEWS 21	FEB 23	Three million new patent records blast AEROSPACE into STN patent clusters
NEWS 22	FEB 25	USGENE enhanced with patent family and legal status display data from INPADOCDB
NEWS 23	MAR 06	INPADOCDB and INPAFAMDB enhanced with new display formats

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,

AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:23:34 ON 10 MAR 2009

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.44 0.44

FILE 'REGISTRY' ENTERED AT 16:24:30 ON 10 MAR 2009
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STRUCTURE FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0
DICTIONARY FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0

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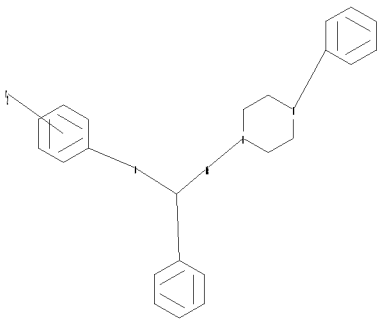
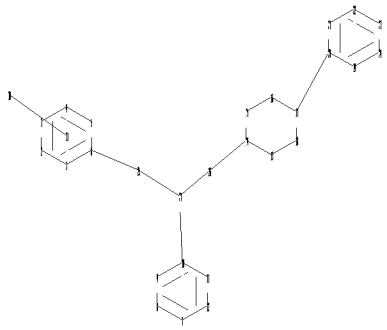
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10594105restriction.str





chain nodes :
25 26 27 30
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-27 14-26 17-20 25-27 26-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 13-14 13-18 14-15 14-26 15-16 16-17 17-18 17-20 25-27 26-27
exact bonds :
10-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

G1:C,N

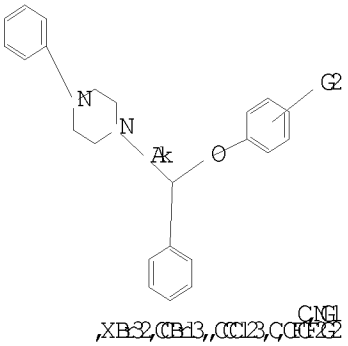
G2:CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 30:CLASS
31:Atom

<12/04/2007> Erich Leese

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 16:25:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 10796 TO ITERATE

100.0% PROCESSED 10796 ITERATIONS 116 ANSWERS
SEARCH TIME: 00.00.02

L2 116 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	186.36	186.80

FILE 'CAPLUS' ENTERED AT 16:25:35 ON 10 MAR 2009
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FILE COVERS 1907 - 10 Mar 2009 VOL 150 ISS 11

FILE LAST UPDATED: 9 Mar 2009 (20090309/ED)

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substance identification.

=> s l2 full
L3   10 L2

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.50	188.30

FILE 'REGISTRY' ENTERED AT 16:27:34 ON 10 MAR 2009
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STRUCTURE FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0
DICTIONARY FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0

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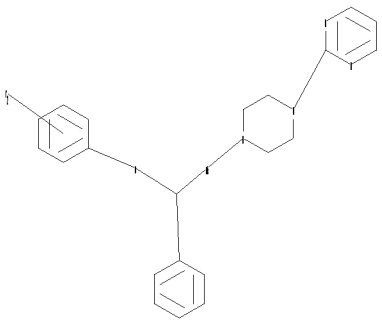
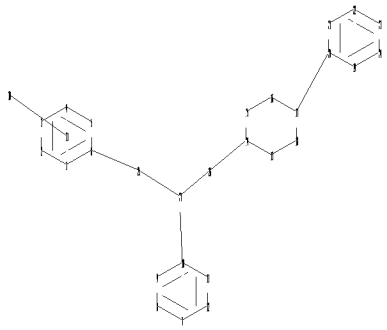
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10594105pyrimidine.str





chain nodes :
25 26 27 30
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-27 14-26 17-20 25-27 26-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 13-14 13-18 14-15 14-26 15-16 16-17 17-18 17-20 25-27 26-27
exact bonds :
10-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

G1:C,N

G2:CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 30:CLASS
31:Atom

<12/04/2007> Erich Leese

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> d l4
L4 HAS NO ANSWERS
L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l4 full
FULL SEARCH INITIATED 16:28:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 267 TO ITERATE

100.0% PROCESSED 267 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L5 6 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 374.18

FILE 'CAPLUS' ENTERED AT 16:28:26 ON 10 MAR 2009
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=> s l5 full
L6 6 L5

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.00	376.18

FILE 'REGISTRY' ENTERED AT 16:30:33 ON 10 MAR 2009
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STRUCTURE FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0
DICTIONARY FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0

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http://www.cas.org/support/stngen/stndoc/properties.html

=>
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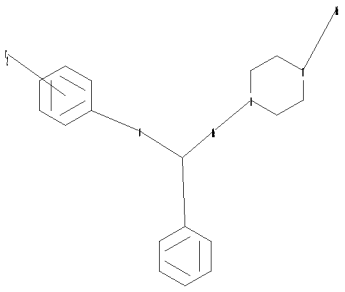
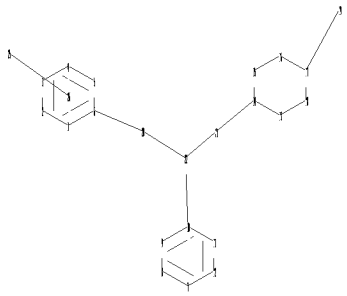




chain nodes :
19 20 21 22 25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
6-20 10-22 14-21 17-19 20-22 21-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18
exact/norm bonds :
6-20 13-14 13-18 14-15 14-21 15-16 16-17 17-18 17-19 20-22 21-22
exact bonds :
10-22
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

G1:C,N

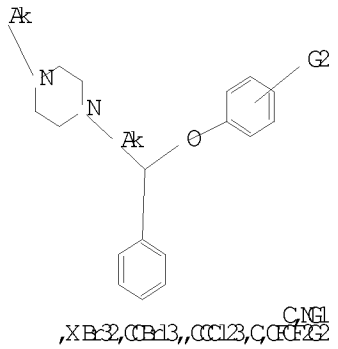
G2:CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 25:CLASS 26:Atom

L7 STRUCTURE UPLOADED

<12/04/2007> Erich Leese

=> d l7
L7 HAS NO ANSWERS
L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l7 full
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FULL SCREEN SEARCH COMPLETED - 69180 TO ITERATE

100.0% PROCESSED 69180 ITERATIONS 74 ANSWERS
SEARCH TIME: 00.00.02

L8 74 SEA SSS FUL L7

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 562.06

FILE 'CAPLUS' ENTERED AT 16:31:15 ON 10 MAR 2009
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=> s l8 full
L9 8 L8

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.50	564.56

FILE 'REGISTRY' ENTERED AT 16:34:04 ON 10 MAR 2009
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DICTIONARY FILE UPDATES: 9 MAR 2009 HIGHEST RN 1118246-54-0

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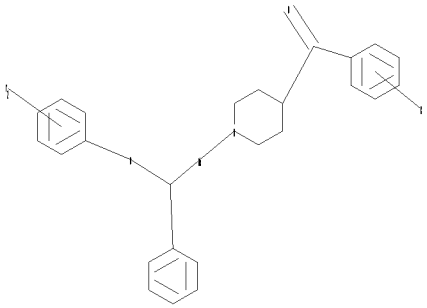
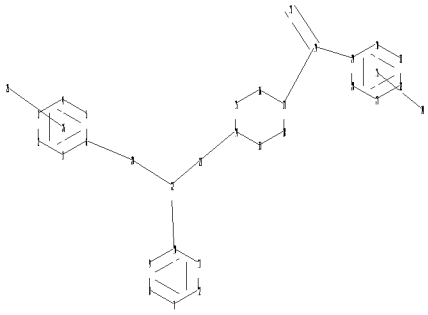
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10594105piperidine.str





chain nodes :
19 20 21 22 25 33 34
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 27 28 29 30 31
32
chain bonds :
6-20 10-22 14-21 17-19 19-29 19-33 20-22 21-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 27-28 27-32 28-29 29-30 30-31 31-32
exact/norm bonds :
6-20 13-14 13-18 14-15 14-21 15-16 16-17 17-18 19-33 20-22 21-22
exact bonds :
10-22 17-19 19-29
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 27-28 27-32
28-29 29-30 30-31 31-32
isolated ring systems :
containing 27 :

G1:C,N

G2:CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:CLASS 33:CLASS 34:CLASS 35:Atom

L10 STRUCTURE UPLOADED

=> s l10 full
FULL SEARCH INITIATED 16:34:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 847 TO ITERATE

100.0% PROCESSED 847 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L11 6 SEA SSS FUL L10

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 186.36 750.92

FILE 'CAPLUS' ENTERED AT 16:35:00 ON 10 MAR 2009
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FILE COVERS 1907 - 10 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 9 Mar 2009 (20090309/ED)

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=> s l11 full
L12 2 L11

=> s l12 or l9 or l6 or l3
L13 16 L12 OR L9 OR L6 OR L3

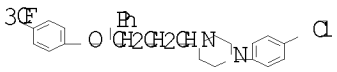
=> d ibib abs hitstr tot

L13 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:803320 CAPLUS
DOCUMENT NUMBER: 149:215113
TITLE: Two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT1A receptor ligands
AUTHOR(S): Weber, Karen C.; Honorio, Kathia M.; Andricopulo, Adriano D.; Da Silva, Alberico B. F.
CORPORATE SOURCE: Instituto de Quimica de Sao Carlos, Universidade de Sao Paulo, Sao Carlos, 13560-970, Brazil
SOURCE: Medicinal Chemistry (2008), 4(4), 328-335
CODEN: MCEHAJ; ISSN: 1573-4064
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

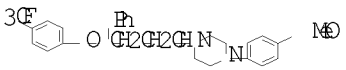
AB 5-HT1A receptor plays an important role in the delayed onset of antidepressant action of a class of selective serotonin reuptake inhibitors. Moreover, 5-HT1A receptor levels have been shown to be altered in patients suffering from major depression. In this work, hologram quant. structure-activity relationship (HQSAR) studies were performed on a series of arylpiperazine compds. presenting affinity to the 5-HT1A receptor. The models were constructed with a training set of 70 compds. The most significant HQSAR model (q2 = 0.81, r2 = 0.96) was generated using atoms, bonds, connections, chirality, and donor and acceptor as fragment distinction, with fragment size of 6-9. Predictions for an external test set containing 20 compds. are in good agreement with exptl. results showing the robustness of the model. Addnl., useful information can be obtained from the 2D contribution maps.

IT ***328248-15-3*** ***328248-21-1*** ***328248-23-3***
328248-24-4 ***328248-30-2*** ***328248-36-8***
753439-74-6 ***767277-20-3*** ***777843-82-0***
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT1A receptor ligands)

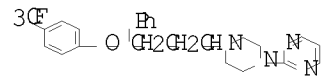
RN 328248-15-3 CAPLUS
CN Piperazine, 1-(4-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



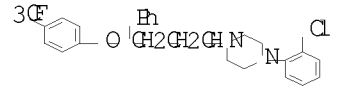
RN 328248-21-1 CAPLUS
CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



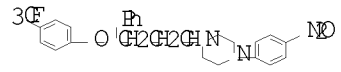
RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



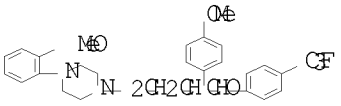
RN 328248-24-4 CAPLUS
CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



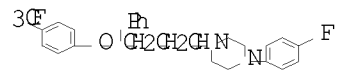
RN 328248-30-2 CAPLUS
CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



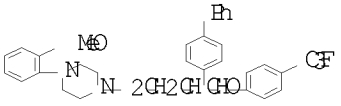
RN 328248-36-8 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



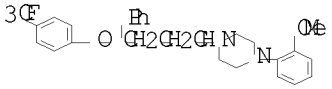
RN 753439-74-6 CAPLUS
CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 767277-20-3 CAPLUS
CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)

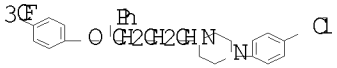


RN 777843-82-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

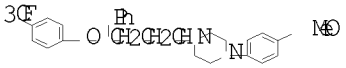


REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

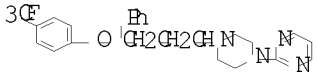
L13 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:767635 CAPLUS
DOCUMENT NUMBER: 149:324283
TITLE: Quantitative structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method
AUTHOR(S): Kuz'min, V. E.; Polischuk, P. G.; Artemenko, A. G.; Makan, S. Yu.; Andronati, S. A.
CORPORATE SOURCE: A.V. Bogatsky Physical-Chemical Institute, National Academy of Sciences of Ukraine, Odessa, Ukraine
SOURCE: SAR and QSAR in Environmental Research (2008), 19(3-4), 213-244
CODEN: SQERED; ISSN: 1062-936X
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The influence of mol. structure of 346 ligands on their affinity for 5-HT1A receptors was investigated. It was shown that the effectiveness of the proposed novel approach for interpretation of decision tree models compared favorably with the PLS method. In the context of the proposed approach, mol. fragments and their values of the relative influence on the affinity for 5-HT1A receptors were defined.
IT ***328248-15-3*** ***328248-21-1*** ***328248-23-3***
328248-24-4 ***328248-30-2*** ***328248-36-8***
753439-74-6 ***767277-20-3*** ***777843-82-0***
RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study)
(quant. structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method)
RN 328248-15-3 CAPLUS
CN Piperazine, 1-(4-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-21-1 CAPLUS
CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

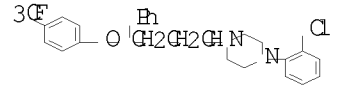


RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)

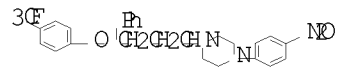


RN 328248-24-4 CAPLUS

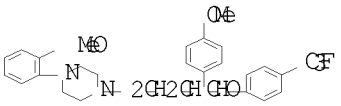
CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



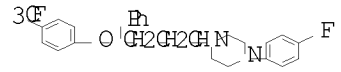
RN 328248-30-2 CAPLUS
CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



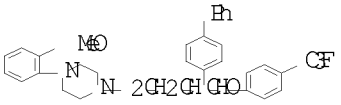
RN 328248-36-8 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



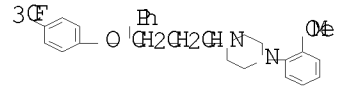
RN 753439-74-6 CAPLUS
CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 767277-20-3 CAPLUS
CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 777843-82-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

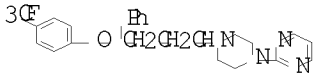
L13 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:232006 CAPLUS
DOCUMENT NUMBER: 148:440268
TITLE: A chemometric study of the 5-HT1A receptor affinities presented by arylpiperazine compounds
AUTHOR(S): Weber, Karen C.; da Silva, Alberico B. F.
CORPORATE SOURCE: Instituto de Quimica de Sao Carlos, Universidade de Sao Paulo, Sao Carlos, 13566-590, Brazil
SOURCE: European Journal of Medicinal Chemistry (2008), 43(2), 364-372
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Masson SAS
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Arylpiperazine compds. are promising 5-HT1A receptor ligands that can contribute for accelerating the onset of therapeutic effect of selective serotonin reuptake inhibitors. In the present work, the chemometric methods HCA, PCA, KNN, SIMCA and PLS were employed in order to obtain SAR and QSAR models relating the structures of arylpiperazine compds. to their 5-HT1A receptor affinities. A training set of 52 compds. was used to construct the models and the best ones were obtained with nine topol. descriptors. The classification and regression models were externally validated by means of predictions for a test set of 14 compds. and have presented good quality, as verified by the correctness of classifications, in the case of pattern recognition studies, and by the high correlation coeffs. (q2 = 0.76, r2 = 0.83) and small prediction errors for the PLS regression. Since the results are in good agreement with previous SAR studies, we can suggest that these findings can help in the search for 5-HT1A receptor ligands that are able to improve antidepressant treatment.

IT ***328248-21-1*** ***328248-23-3*** ***328248-24-4***
328248-30-2 ***328248-36-8*** ***753439-74-6***
767277-20-3 ***777843-82-0***
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(chemometric study of 5-HT1A receptor affinities presented by arylpiperazine compds. as possible antidepressants)

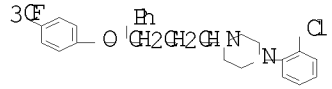
RN 328248-21-1 CAPLUS
CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)

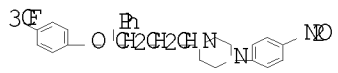


RN 328248-24-4 CAPLUS
CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-

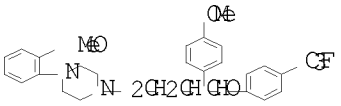
(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



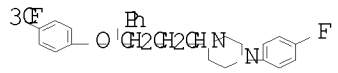
RN 328248-30-2 CAPLUS
CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



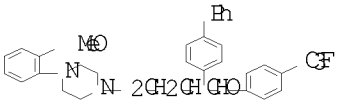
RN 328248-36-8 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



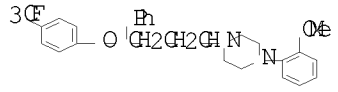
RN 753439-74-6 CAPLUS
CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 767277-20-3 CAPLUS
CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



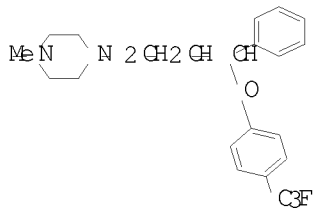
RN 777843-82-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:847178 CAPLUS
DOCUMENT NUMBER: 145:410017
TITLE: Synthesis of benzenepropanamine analogues as non-detergent spermicides with antitrichomonas and anticandida activities
AUTHOR(S): Kumar, S. T. V. S. Kiran; Sharma, Vishnu Lal; Kumar, Manish; Shukla, Praveen Kumar; Tiwari, Pratibha; Jain, Rajeev Kumar; Maikhuri, Jagdamba Prasad; Singh, Divya; Gupta, Gopal; Singh, Man Mohan
CORPORATE SOURCE: Division of Medicinal and Process Chemistry, Central Drug Research Institute, Lucknow, 226001, India
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(19), 6593-6600
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:410017
GI



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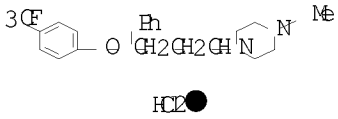
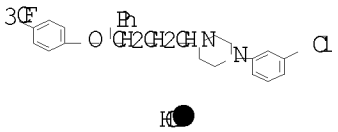
AB Fifteen analogs of benzenepropanamine were synthesized and evaluated for their spermicidal as well as microbicidal activities against Trichomonas vaginalis and Candida spp. Several compds. showed appreciable dual activities. Compound I exhibited good spermicidal (MEC = 0.1%) along with substantial anticandidal (MIC = 0.05%) activities, while compds. 3 and 6 showed significant microbicidal activities with moderate spermicidal effect. The SAR of these structures is being discussed here in this communication. It is concluded that suitable structural modifications in this class of compds. at 3-amino position may lead to a potent spermicide with associated microbicidal activity.

IT ***911811-07-9P*** ***911811-08-0P*** ***911811-09-1P*** ***911811-11-5P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(benzenepropanamine analogs as non-detergent spermicides with antitrichomonas and anticandida activities)

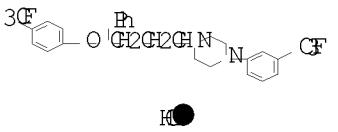
RN 911811-07-9 CAPLUS
CN Piperazine, 1-methyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)



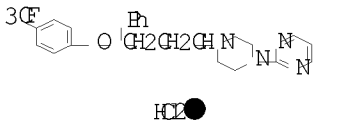
RN 911811-08-0 CAPLUS
CN Piperazine, 1-(3-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:1) (CA INDEX NAME)



RN 911811-09-1 CAPLUS
CN Piperazine, 1-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



RN 911811-11-5 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1289687 CAPLUS
DOCUMENT NUMBER: 144:51568
TITLE: Preparation of substituted 2-quinolyl-oxazoles and their heterocyclic analogs useful as pde4 inhibitors
INVENTOR(S): Kuang, Rongze; Blythin, David; Shih, Neng-Yang; Shue, Ho-Jane; Chen, Xiao; Cao, Jianhua; Gu, Danlin; Huang, Ying; Schwerdt, John H.; Ting, Pauline C.; Wong, Shing-Chun; Xiao, Li
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 233 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005116009	A1	20051208	WO 2005-US17134	20050516
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005247906	A1	20051208	AU 2005-247906	20050516
CA 2565599	A1	20051208	CA 2005-2565599	20050516
US 20060106062	A1	20060518	US 2005-130359	20050516
EP 1758883	A1	20070307	EP 2005-750076	20050516
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CN 1984901	A	20070620	CN 2005-80023666	20050516
BR 2005011295	A	20071204	BR 2005-11295	20050516
JP 2007537300	T	20071220	JP 2007-513471	20050516
TW 286475	B	20070911	TW 2005-94115924	20050517
MX 2006013414	A	20070123	MX 2006-13414	20061117
KR 2007013306	A	20070130	KR 2006-724186	20061117
IN 2006CN04254	A	20070629	IN 2006-CN4254	20061117
NO 2006005830	A	20070216	NO 2006-5830	20061215

PRIORITY APPLN. INFO.: US 2004-572266P P 20040518
WO 2005-US17134 W 20050516
OTHER SOURCE(S): CASREACT 144:51568; MARPAT 144:51568
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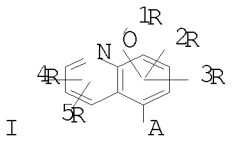

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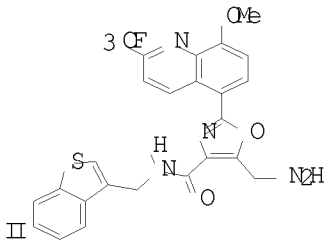


II

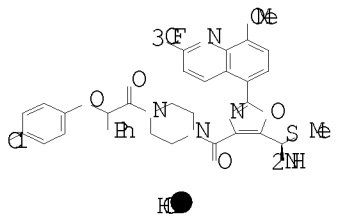
AB Title compds. I [R1 = H, alkyl, cycloalkyl; R2, R3 and R5 independently = H or halo; R4 = H, halo, alkyl, etc.; A = substituted oxazolyl, imidazole, thiazole or pyrrole], and their pharmaceutically acceptable salts, are prepared and disclosed as pde4 inhibitors. Thus, e.g., II was prepared in a multistep synthesis from 2-trifluoromethyl-8-methoxyquinolin-5-yl carboxylic acid. In PDE4 assays, selected compds. possessed IC50 values ranging from 0.01-1.8 nM. Also claimed are pharmaceutical compns., the use of the compds. as PDE4 inhibitors, and combinations with other actives.

IT ***871009-78-8P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted quinolyloxazoles and their heterocyclic analogs useful as PDE4 inhibitors)

RN 871009-78-8 CAPLUS

CN Ethanone, 1-[4-[[5-[(1S)-1-aminoethyl]-2-[8-methoxy-2-(trifluoromethyl)-5-quinolinyl]-4-oxazolyl]carbonyl]-1-piperazinyl]-2-(4-chlorophenoxy)-2-phenyl-, hydrochloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.

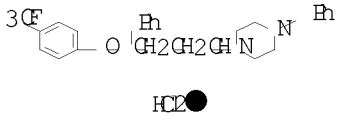


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

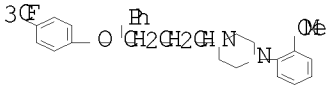
L13 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1143268 CAPLUS
DOCUMENT NUMBER: 144:63874
TITLE: Design and synthesis of long-chain arylpiperazines with mixed affinity for serotonin transporter (SERT) and 5-HT1A receptor
AUTHOR(S): Perrone, Roberto; Berardi, Francesco; Colabufo, Nicola A.; Lacivita, Enza; Larizza, Carmela; Leopoldo, Marcello; Tortorella, Vincenzo
CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita degli Studi di Bari, Bari, 70125, Italy
SOURCE: Journal of Pharmacy and Pharmacology (2005), 57(10), 1319-1327
CODEN: JPPMAB; ISSN: 0022-3573
PUBLISHER: Pharmaceutical Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:63874

AB A new generation of antidepressant agents could be represented by compds. with mixed activity as serotonin transporter (SERT) inhibitors and 5-HT1A receptor antagonists. We report here on the synthesis and evaluation of SERT and 5-HT1A receptor affinity of long-chain arylpiperazines obtained either by modifying 6-nitroquipazine into a long-chain arylpiperazine or by inserting a modified 6-nitroquipazine moiety or other structures endowed with SERT affinity into a long-chain arylpiperazine with 5-HT1A affinity. Among the compds. studied, 2-[4-(2-methoxyphenyl)piperazin-1-yl]-N-(6-nitro-2-quinolyl)ethylamine (21) and 1-(5-bromo-1,2,3,4-tetrahydronaphthalen-1-yl)-3-[4-(2-methoxyphenyl)-piperazin-1-yl]-1-propanone (24) showed good affinity values for SERT and 5-HT1A receptors (SERT: Ki (inhibition constant) = 71.8 and 62.8 nM; 5-HT1A Ki = 14.2 and 0.82 nM, resp.).

IT ***871739-17-2P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(arylpiperazines with mixed affinity for serotonin transporter and 5-HT1A receptor)
RN 871739-17-2 CAPLUS
CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)



IT ***777843-82-0***
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(arylpiperazines with mixed affinity for serotonin transporter and 5-HT1A receptor)
RN 777843-82-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

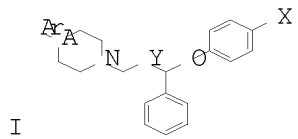


REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

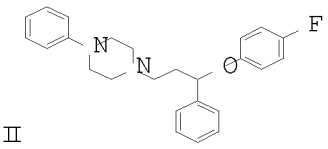
L13 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103625 CAPLUS
DOCUMENT NUMBER: 143:387060
TITLE: Preparation of piperazine or piperidine derivatives as serotonin reuptake inhibitors
INVENTOR(S): Pinney, Kevin G.; Miranda, Maria Graciela; Dorsey, James Michael
PATENT ASSIGNEE(S): Baylor University, USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005094896	A2	20051013	WO 2005-US10356	20050328
WO 2005094896	A3	20070503		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AP, EA, EP, OA				
EP 1732610	A2	20061220	EP 2005-730778	20050328
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
US 20080132514	A1	20080605	US 2007-594105	20070921

PRIORITY APPLN. INFO.: US 2004-557069P P 20040326
WO 2005-US10356 W 20050328
OTHER SOURCE(S): CASREACT 143:387060; MARPAT 143:387060
GI



I



II

AB Title compds. I [X = F or CF3; Y = (CH2)n; n = 0-1; A = N or C; Ar = aryl] and their pharmaceutically acceptable salts, are prepared and disclosed as serotonin reuptake inhibitors. Thus, e.g., II was prepared by reduction of 1-phenyl-3-(4-phenyl-piperazin-1-yl)-propan-1-ol (preparation given) using sodium borohydride followed by coupling with 4-fluorophenol. The ability of I to inhibit [3H]5-HT uptake was evaluated using liquid scintillation spectroscopy and it was revealed that selected compds. of the invention possessed IC50 values in the range of